

QUANTUM WAVEGUIDES WITH SMALL PERIODIC PERTURBATIONS: GAPS AND EDGES OF BRILLOUIN ZONES

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ABSTRACT. We consider small perturbations of the Laplace operator in a multi-dimensional cylindrical domain by second order differential operators with periodic coefficients. We show that under certain non-degeneracy conditions such perturbations can open a gap in the continuous spectrum and give the leading asymptotic terms for the gap edges. We also estimate the values of quasi-momentum at which the spectrum edges are attained. The general machinery is illustrated by several new examples in two- and three-dimensional structures.

1. INTRODUCTION

This paper is devoted to the spectral problem for a class of periodic differential operators in unbounded periodic domains. The spectra of such operators are known to have band structure, and one is interested in the question whether the spectrum fills a semi-axis or has gaps. The importance of such questions is motivated, in particular, by the study of photonic crystals [1]: the spectral gaps correspond to the energies at which no photons can be transmitted through the material.

Existence of gaps for various periodic operators attracted a lot of attention in the last decade, see e.g. the reviews [2, 3]. We mention, in particular, the recent papers [4, 5, 6] discussing gap opening for tube-type domains with various perturbations. Our interest to the problem was attracted by the paper [7, 8], in which the authors discussed the locations of the extrema of the band functions inside the Brillouin zone for generic periodic operators. In particular, the paper [8] was devoted specifically to the operators with the one-dimensional periodicity, and it was shown that the spectral edges are generically different from the periodic and the anti-periodic eigenvalues as it is sometimes assumed. One of the most natural classes of one-periodic systems is provided by the waveguides, but it seems that there are just few works addressing the related questions. The paper [9] discussed the spectra of acoustic structures, and our papers [10, 11] showed the occurrence of the same effect for a configuration consisting of two interacting waveguides modeled by the free Laplacian, and this discussion was continued in the very recent work [12] at the example of a cylinder with a periodic system of holes. We mention another recent paper [13] discussing related questions at the physical level of rigor.

In the present paper we prove a general result giving sufficient conditions for the gap opening for a class of second-order operators in multi-dimensional cylindrical domains. It is shown that the presence of gaps at the energies different from the periodic and anti-periodic eigenvalues is a generic fact, and we discuss the parameters controlling the gap opening at various values of the quasi-momentum. Like in [10, 11, 12], the gap opening may occur at the points where the band functions of the reference operator (the free Laplacian) meet in some specific way, but the further analysis is done with the help of the elementary tools of the regular first-order perturbation theory, while the previous works used singular asymptotic expansions or other methods which are rather sensible to the type of perturbation. We discuss in detail several new examples and show that the gaps at the interior points of

the Brillouin zone and at its center are controlled by different parameters. In particular, we put in evidence several perturbations which open gaps at intermediate values of the quasimomentum, but the leading asymptotic term appears to vanish at the center of the Brillouin zone. Therefore, our analysis considerably extends the family of situations for which one can prove the existence of gaps compared to the previous works.

2. FORMULATION OF THE PROBLEM AND THE MAIN RESULT

Let $x' = (x_1, \dots, x_{n-1})$, $x = (x', x_n)$ be Cartesian coordinates in \mathbb{R}^{n-1} and \mathbb{R}^n , respectively, $n \geq 2$, and ω be a connected bounded domain in \mathbb{R}^{n-1} with Lipschitz boundary. By Ω we denote an infinite straight cylinder in \mathbb{R}^n with the base ω , namely, $\Omega := \omega \times \mathbb{R}$, and by \mathcal{H}_0 we denote the positive Dirichlet Laplacian in $L_2(\Omega)$ on the domain $\dot{W}_2^2(\Omega)$, which is introduced as the subspace of the functions in $W_2^2(\Omega)$ with zero trace on $\partial\Omega$. We assume that the boundary $\partial\omega$ is sufficiently regular for the operator \mathcal{H}_0 to be self-adjoint in $L_2(\Omega)$. Introduce another differential operator \mathcal{L}_ε with the domain $\dot{W}_2^2(\Omega)$ whose coefficients may depend on a small positive parameter ε ,

$$\mathcal{L}_\varepsilon := - \sum_{i,j=1}^n \frac{\partial}{\partial x_i} A_{ij} \frac{\partial}{\partial x_j} + i \sum_{j=1}^n \left(A_j \frac{\partial}{\partial x_j} + \frac{\partial}{\partial x_j} A_j \right) + A_0,$$

where $A_{ij} \in W_\infty^1(\Omega)$ are complex-valued functions satisfying $A_{ij} = \overline{A_{ji}}$, and $A_j \in W_\infty^1(\Omega)$, $A_0 \in L_\infty(\Omega)$ are real-valued functions. All the coefficients are supposed to be T -periodic in x_n :

$$\begin{aligned} A_{ij}(x', x_n + T, \varepsilon) &= A_{ij}(x, \varepsilon), & i, j &= 1, \dots, n, \\ A_j(x', x_n + T, \varepsilon) &= A_j(x, \varepsilon), & j &= 0, \dots, n, \end{aligned}$$

with an ε -independent period T . We assume that for $\varepsilon \rightarrow +0$ one has

$$\begin{aligned} \sum_{i,j=1}^n \|A_{ij}(\cdot, \varepsilon) - A_{ij}(\cdot, 0)\|_{W_\infty^1(\square)} + \sum_{j=1}^n \|A_j(\cdot, \varepsilon) - A_j(\cdot, 0)\|_{W_\infty^1(\square)} \\ + \|A_0(\cdot, \varepsilon) - A_0(\cdot, 0)\|_{L_\infty(\square)} =: \eta(\varepsilon) \rightarrow +0, \end{aligned} \quad (2.1)$$

where $\square := \omega \times (0, T)$ is the elementary cell. The condition (2.1) is satisfied, if, for example, all the coefficients are continuously differentiable in both x and ε .

Under the above assumptions and for sufficiently small ε the operator \mathcal{L}_ε is symmetric and relatively bounded w.r.t. \mathcal{H}_0 , and, by Kato-Rellich theorem, for small ε one can define the sum $\mathcal{H}_\varepsilon := \mathcal{H}_0 + \varepsilon \mathcal{L}_\varepsilon$ which is a self-adjoint operator in $L_2(\Omega)$. One can consider \mathcal{H}_ε as the Hamiltonian of a quantum particle in the waveguide Ω .

Due to the periodicity, the operator \mathcal{H}_ε can be studied using the Floquet-Bloch theory [14]. Introduce self-adjoint operators

$$\mathcal{H}_\varepsilon(\tau) := -\Delta_{x'} + \left(i \frac{\partial}{\partial x_n} - \tau \right)^2 + \varepsilon \mathcal{L}_\varepsilon(\tau), \quad (2.2)$$

$$\mathcal{L}_\varepsilon(\tau) := \sum_{i,j=1}^n l_i(\tau) A_{ij} l_j(\tau) + \sum_{j=1}^n (A_j l_j(\tau) + l_j(\tau) A_j) + A_0, \quad (2.3)$$

$$l_j(\tau) := i \frac{\partial}{\partial x_j}, \quad j = 1, \dots, n-1, \quad l_n(\tau) := i \frac{\partial}{\partial x_n} - \tau,$$

depending on the parameter $\tau \in \mathcal{B} = (-\pi/T, \pi/T]$ and acting in $L_2(\square)$ on the domain $\dot{W}_{2,per}^2(\square)$ consisting of the functions from $W_2^2(\square)$ with zero trace on $\partial\omega \times (0, T)$ and satisfying periodic boundary condition at $x_n = 0$ and $x_n = T$. The

parameter τ is referred to as the *quasi-momentum* and the set \mathcal{B} is usually called the *Brillouin zone*.

For any τ , the operator $\mathcal{H}_\varepsilon(\tau)$ has a compact resolvent, and its spectrum consists of an infinite sequence of discrete real eigenvalues $E_m(\tau, \varepsilon)$, $m \geq 1$, which we assume to be ordered in the ascending order counting multiplicity. The mappings $\tau \mapsto E_m(\tau, \varepsilon)$ are called *band functions*; it is known that they are continuous with $E_m(-\pi/T, \varepsilon) = E_m(\pi/T, \varepsilon)$ and that the spectrum of \mathcal{H}_ε is the union of their ranges,

$$\sigma(\mathcal{H}_\varepsilon) = \bigcup_{m=1}^{\infty} \{E_m(\tau, \varepsilon) : \tau \in \mathcal{B}\}.$$

In particular, $\inf \sigma(\mathcal{H}_\varepsilon) = \Sigma_\varepsilon = \min_{\tau \in \mathcal{B}} E_1(\tau, \varepsilon)$. Each open interval $(\alpha, \beta) \subset [\Sigma_\varepsilon, +\infty) \setminus \sigma(\mathcal{H}_\varepsilon)$ with $\alpha, \beta \in \sigma(\mathcal{H}_\varepsilon)$ is called a *gap* of \mathcal{H}_ε . We note that the unperturbed operator \mathcal{H}_0 has no gaps and its spectrum fills a semi-axis (see below). We also observe that the band functions are not constant on any interval, and the spectrum of \mathcal{H}_ε is absolutely continuous [15, 16, 17, 18]. The main aim of the present paper is to obtain some conditions guaranteeing the existence of gaps for \mathcal{H}_ε and to determine the values of the quasi-momentum τ at which the band functions attain the respective gap edges α and β .

The eigenvalues of $\mathcal{H}_0(\tau)$ can be found by the separation of variables. Denote by $-\Delta_\omega^{(D)}$ the positive Dirichlet Laplacian in ω . Since this operator is self-adjoint and has a compact resolvent, its spectrum consists of real eigenvalues of finite multiplicity denoted by λ_j , $j = 1, 2, \dots$, and assumed to be ordered in the ascending order counting multiplicity. The spectrum of $\mathcal{H}_0(\tau)$ then consists of the eigenvalues

$$\Lambda_{j,p}(\tau) = \lambda_j + \left(\tau + \frac{2\pi p}{T} \right)^2, \quad j \in \mathbb{N}, \quad p \in \mathbb{Z}, \quad (2.4)$$

and the values $E_m(\tau, 0)$ are obtained by their rearrangement in the ascending order. Moreover, if $\psi_j(x')$ are the eigenfunctions of $-\Delta_\omega^{(D)}$ associated with the eigenvalues λ_j and chosen real and orthonormal, then the eigenfunctions $\Psi_{j,p}$ of $\mathcal{H}_0(\tau)$ for the eigenvalues $\Lambda_{j,p}(\tau)$ can be written as

$$\Psi_{j,p}(x) := \frac{1}{T^{1/2}} \psi_j(x') e^{\frac{2\pi i p}{T} x_n}, \quad (2.5)$$

and they are orthonormal in $L_2(\square)$. Let us formulate our main result.

Theorem 2.1. *Let numbers $\tau_0 \in \left[0, \frac{\pi}{T}\right]$, $j, k \in \{1, 2\}$ and $p, q \in \mathbb{Z}$ satisfy the following conditions:*

$$\lambda_j \text{ and } \lambda_k \text{ are simple eigenvalues of } -\Delta_\omega^{(D)}; \quad (2.6)$$

$$\Lambda_{j,p}(\tau_0) = \Lambda_{k,q}(\tau_0) =: \Lambda_0; \quad (2.7)$$

$$\frac{\partial \Lambda_{j,p}}{\partial \tau}(\tau_0) \frac{\partial \Lambda_{k,q}}{\partial \tau}(\tau_0) < 0; \quad (2.8)$$

$$\Lambda_0 \notin \Lambda_{l,s} \left(\left[0, \frac{\pi}{T}\right] \right) \text{ as } (l, s) \notin \{(j, p), (k, q)\}; \quad (2.9)$$

$$\langle \mathcal{L}_0(\pm \tau_0) \Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} \neq 0. \quad (2.10)$$

Define the functions

$$\beta_\pm(\tau) := \pm \frac{|b_{12}^0(\tau)|}{|k_3(\tau)|} \sqrt{k_3^2(\tau) - k_1^2(\tau)} - \frac{k_1(\tau)k_4(\tau)}{k_3(\tau)} + k_2(\tau), \quad (2.11)$$

where

$$\begin{aligned} k_1(\tau) &:= -\frac{\pi(p+q)}{T} - \tau, \quad k_2(\tau) := -\frac{b_{11}^0(\tau) + b_{22}^0(\tau)}{2}, \\ k_3(\tau) &:= \frac{\pi}{T}(p-q), \quad k_4(\tau) := \frac{b_{22}^0(\tau) - b_{11}^0(\tau)}{2}. \end{aligned} \quad (2.12)$$

$$B_0(\tau) := \begin{pmatrix} b_{11}^0(\tau) & b_{12}^0(\tau) \\ b_{21}^0(\tau) & b_{22}^0(\tau) \end{pmatrix} = \begin{pmatrix} \langle \mathcal{L}_0(\tau) \Psi_{j,p}, \Psi_{j,p} \rangle_{L_2(\square)} & \langle \mathcal{L}_0(\tau) \Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} \\ \langle \mathcal{L}_0(\tau) \Psi_{k,q}, \Psi_{j,p} \rangle_{L_2(\square)} & \langle \mathcal{L}_0(\tau) \Psi_{k,q}, \Psi_{k,q} \rangle_{L_2(\square)} \end{pmatrix}, \quad (2.13)$$

as $\tau \geq 0$, and

$$k_1(\tau) := \frac{\pi(p+q)}{T} - \tau, \quad k_2(\tau) := -\frac{b_{11}^0(\tau) + b_{22}^0(\tau)}{2}, \quad (2.14)$$

$$k_3(\tau) := \frac{\pi}{T}(q-p), \quad k_4(\tau) := \frac{b_{22}^0(\tau) - b_{11}^0(\tau)}{2}.$$

$$B_0(\tau) := \begin{pmatrix} b_{11}^0(\tau) & b_{12}^0(\tau) \\ b_{21}^0(\tau) & b_{22}^0(\tau) \end{pmatrix} \quad (2.15)$$

$$= \begin{pmatrix} \langle \mathcal{L}_0(\tau) \Psi_{j,-p}, \Psi_{j,-p} \rangle_{L_2(\square)} & \langle \mathcal{L}_0(\tau) \Psi_{j,-p}, \Psi_{k,-q} \rangle_{L_2(\square)} \\ \langle \mathcal{L}_0(\tau) \Psi_{k,-q}, \Psi_{j,-p} \rangle_{L_2(\square)} & \langle \mathcal{L}_0(\tau) \Psi_{k,-q}, \Psi_{k,-q} \rangle_{L_2(\square)} \end{pmatrix}, \quad (2.16)$$

as $\tau < 0$. Then

(A1) The strict inequalities $\beta_-(\tau_0) < \beta_+(\tau_0)$ and $\beta_-(-\tau_0) < \beta_+(-\tau_0)$ hold true.

(A2) If, in addition, one has

$$\beta_l := \max\{\beta_-(\tau_0), \beta_-(-\tau_0)\} < \beta_r := \min\{\beta_+(\tau_0), \beta_+(-\tau_0)\}, \quad (2.17)$$

then there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$ the operator \mathcal{H}_ε has a spectral gap $(\alpha_l(\varepsilon), \alpha_r(\varepsilon))$ whose edges have the asymptotics

$$\alpha_{l/r}(\varepsilon) = \Lambda_0 + \varepsilon \beta_{l/r} + \mathcal{O}(\varepsilon^2 + \varepsilon \eta(\varepsilon)), \quad (2.18)$$

and the associated band functions $E_{l/r}(\varepsilon, \tau)$ of \mathcal{H}_ε attain the gap edges $\alpha_{l/r}(\varepsilon)$ at the points $\tau_{l/r}(\varepsilon)$,

$$\min_{\tau} E_r(\varepsilon, \tau) = E_r(\varepsilon, \tau_r(\varepsilon)), \quad \min_{\tau} E_l(\varepsilon, \tau) = E_l(\varepsilon, \tau_l(\varepsilon)), \quad (2.19)$$

for which the asymptotics

$$\tau_{l/r}(\varepsilon) = \tau_0 + \varepsilon \gamma_{l/r} + \mathcal{O}(\varepsilon^{3/2} + \varepsilon \eta^{1/2}) \quad (2.20)$$

$$\begin{aligned} \gamma_l &:= \frac{k_1(\tau_*)|b_{12}^0(\tau_*)|}{|k_3(\tau_*)|\sqrt{k_3(\tau_*)^2 - k_1^2(\tau_*)}} - \frac{k_4(\tau_*)}{k_3(\tau_*)}, \\ \gamma_r &:= -\frac{k_1(\tau_*)|b_{12}^0(\tau_*)|}{|k_3(\tau_*)|\sqrt{k_3(\tau_*)^2 - k_1^2(\tau_*)}} - \frac{k_4(\tau_*)}{k_3(\tau_*)}, \end{aligned}$$

are valid. In each of the latter formulas the number τ_* should be chosen to that of the values $\pm\tau_0$, at which the maximum or minimum is attained in the formulas (2.17).

(A3) If at least one the following two conditions is valid:

- all the coefficients \mathcal{H}_ε are real
- $\tau_0 = 0$,

then the condition (2.17) is satisfied.

Before proceeding to the proof, let us give some comments on the assumptions and the statement of the theorem.

Remark 2.1. Eq. (2.6) is a non-degeneracy condition. It is independent of the period T and concerns only the eigenvalues of the cross-section operator $-\Delta_\omega^{(D)}$. This condition allows us to reduce the spectral study of \mathcal{H}_ε in a vicinity of Λ_0 to an eigenvalue splitting problem for a 2×2 matrix. Note that this condition is always valid for $j = k = 1$, because the lowest eigenvalue of the Dirichlet Laplacian in a bounded connected domain is always non-degenerate.

Remark 2.2. The conditions (2.7), (2.8) and (2.9) impose some restrictions on the behavior of the band functions $\Lambda_{j,p}$ and $\Lambda_{k,q}$ at the intersection point. The condition (2.7) means exactly the presence of an intersection. The condition (2.8) shows that one of the functions increases and the other decreases at the intersection point. Finally, the third condition (2.9) expresses the fact that the projection of the intersection point on the ordinate axis should not be overlapped by the projections of the graphs of the remaining band functions $\Lambda_{l,s}(\tau)$ as $\tau \in [0, \pi/T]$. We observe that it is possible only as $j + k \leq 3$.

One can easily see that the validity of these assumptions is conditioned by the presence of certain relations between the transversal eigenvalues λ_j and the period T . We remark first that the conditions (2.4) and (2.7) can hold true only for p and q having opposite signs. Moreover, due to (2.4) one has

$$\lambda_k - \lambda_j = \frac{2\pi(p - q)}{T} \left(\frac{2\pi(p + q)}{T} + 2\tau_0 \right). \quad (2.21)$$

In particular, if all three conditions in question can be satisfied with $\tau_0 = 0$ for $j = k = 1$ and $q = -p$ only, and if all the conditions are valid for $\tau_0 = \pi/T$, then automatically $j = k = 1$ and $q = -p - 1$.

To guarantee the presence of at least one combination (j, p) , (k, q) satisfying the above assumptions for $\tau_0 = 0$, it is sufficient to ask for the inequality $\Lambda_{1,1}(0) < \Lambda_{2,0}(0)$, which is equivalent to $T > 2\pi/\sqrt{\lambda_2 - \lambda_1}$; in this case all three conditions are valid for $\tau_0 = 0$, $j = k = 1$, $p = 1$, $q = -1$. On the other hand, to satisfy the conditions (2.7) and (2.8) for some $\tau_0 \in (0, \pi/T)$ it is sufficient to obey, for instance, the inequality $\Lambda_{2,0}(0) < \Lambda_{1,1}(0)$, then one can take $j = 1$, $k = 2$, $p = -1$ and $q = 0$, and the condition (2.9) is equivalent to $\Lambda_{2,0}(\tau_0) < \Lambda_{3,0}(0)$. Rewriting these inequalities with the help of the explicit expressions (2.4), one can easily see that the three conditions (2.7), (2.8), (2.9) hold true with some $\tau_0 \in (0, \pi/T)$, $j = 1$, $k = 2$, $p = -1$ and $q = 0$, if the period T obeys the estimates

$$\frac{2\pi}{\sqrt{\lambda_3 - \lambda_1} - \sqrt{\lambda_3 - \lambda_2}} < T < \frac{2\pi}{\sqrt{\lambda_2 - \lambda_1}}.$$

With the help of the explicit formulas for $\Lambda_{j,p}$ one can easily construct other sufficient conditions. Note that for any fixed cross-section ω one can satisfy the assumption by an appropriate choice of the period T , and, moreover, one can obtain in this way any prescribed finite number of intersections satisfying all the assumptions. One is also able to choose parameters in such a way that the assumption will be satisfied for any prescribed value of τ_0 .

Remark 2.3. The key condition (2.10) allows one to make some conclusions on the behavior of the perturbed band functions in a vicinity of τ_0 using some elementary tools of the regular perturbation theory. Checking this condition is usually the most difficult step when applying the theorem, which will be seen with the series of examples below. As follows from A3, for operators with real-valued coefficients as well as for $\tau_0 = 0$, Eq. (2.10) is the only non-trivial assumption on the perturbation \mathcal{L}_ε .

Remark 2.4. The theorem can be extended to other types of unperturbed operators as far as the unperturbed band functions have a similar structure. We do not develop this direction to avoid technicalities. We just remark that the results are valid in literally the same form for some other boundary conditions $\partial\Omega$, in particular, for the Neumann condition and the Robin condition with a constant coefficient, and such a modification results in an appropriate redefinition of the eigenvalues λ_j and the eigenfunctions ψ_j .

3. PROOF OF THE MAIN RESULT

This section is completely devoted to the proof of Theorem 2.1. We do all the constructions for $\tau_0 \in [0, \pi/T)$ only; the study of $\tau_0 = \pi/T$ is completely identical, but it requires cumbersome notation since it corresponds to the end point of the Brillouin zone.

By (2.1) one can represent $\mathcal{L}_\varepsilon = \mathcal{L}_0 + \eta(\varepsilon)\mathcal{M}_\varepsilon$, where \mathcal{M}_ε the operator is of the same type as \mathcal{L}_ε except the fact that instead of the continuity in ε at $\varepsilon = 0$ we ask for the uniform boundedness for $\varepsilon < \varepsilon_1$ in the appropriate Sobolev norms. Under these assumptions and for sufficiently small ε the operator \mathcal{M}_ε is relatively bounded w.r.t. $\mathcal{K}_\varepsilon := \mathcal{H}_0 + \varepsilon\mathcal{L}_0$. By analogy with (2.3) one can define the operators $\mathcal{M}_\varepsilon(\tau)$ and $\mathcal{K}_\varepsilon(\tau)$, and then $\mathcal{M}_\varepsilon(\tau)$ is also relatively bounded w.r.t. $\mathcal{K}_\varepsilon(\tau)$.

Denote by $\tilde{E}_m(\tau, \varepsilon)$, $m = 1, 2, \dots$, the eigenvalues of $\mathcal{K}_\varepsilon(\tau)$ taken in the ascending order counting multiplicity. By the minimax principle one can choose a constant $c > 0$ such that for sufficiently small ε the uniform in $\tau \in \mathcal{B}$ estimates

$$|E_m(\tau, \varepsilon) - E_m(\tau, 0)| \leq c\varepsilon |E_m(\tau, 0)|, \quad |\tilde{E}_m(\tau, \varepsilon) - E_m(\tau, \varepsilon)| \leq c\varepsilon \eta(\varepsilon) |E_m(\tau, 0)| \quad (3.1)$$

hold true. Since the required estimates in A2 are linear in ε , the second inequality in (3.1) shows that it is sufficient to consider the case of an ε -independent perturbation, $\mathcal{L}_\varepsilon = \mathcal{L}_0$, which will be assumed throughout the rest of the proof.

The explicit expressions show that for any $C > \Lambda_0$ there exists just a finite number of the pairs $(l, s) \in \mathbb{N} \times \mathbb{Z}$ with $(-\infty, C) \cap \Lambda_{l,s}(\mathcal{B}) \neq \emptyset$. Pick an arbitrary $C_1 > \Lambda_0$, then, by (3.1), one can find $N \in \mathbb{N}$ and $\varepsilon_2 > 0$ such that $E_m(\tau, \varepsilon) > C_1$ for all $m > N$, $\varepsilon < \varepsilon_2$ and $\tau \in \mathcal{B}$. Thus, there exists $C_2 > 0$ such that $|E_m(\tau, \varepsilon) - E_m(\tau, 0)| \leq C_2\varepsilon$ for all $m \leq N$, $|\varepsilon| < \varepsilon_2$ and $\tau \in \mathcal{B}$.

Now we find $M \in \mathbb{N}$ for which $\Lambda_0 = E_M(\tau_0, 0) = E_{M+1}(\tau_0, 0)$. By the preceding estimates we can conclude that for any $\delta > 0$ there exists $\varepsilon_3 > 0$ such that $(\Lambda_0 - \delta, \Lambda_0 + \delta) \cap E_j(\mathcal{B}, \varepsilon) = \emptyset$ for all $j \notin \{M, M+1\}$ $|\varepsilon| < \varepsilon_3$. Thus, the spectrum of \mathcal{H}_ε near Λ_0 for small ε is determined by the behavior of the two band functions E_M and E_{M+1} near $\pm\tau_0$, and for $\varepsilon = 0$ they coincide locally with the functions $\Lambda_{j,p}$ and $\Lambda_{k,q}$.

By (2.4) we have $\Lambda_{j,-p}(-\tau) = \Lambda_{j,p}(\tau)$. This shows that the assumptions (2.7), (2.8) and (2.10) are also valid with j, p, k, q and τ_0 replaced by $j, -p, k, -q$ and $-\tau_0$, respectively, and with the same value Λ_0 . One can find a neighborhood of Λ_0 having no intersections with the ranges of $\Lambda_{l,s}$ as $(l, s) \notin \{(j, p), (k, q)\}$ and, moreover, it is clear that in $[-\pi/T, \pi/T]$ there are no other values $\pm\tau_0$ for which Eq. (2.7) holds. To summarize, for $\varepsilon \in (0, \varepsilon_3)$ and for any $a > 0$ there is a constant $t_0(a) > 0$ such that

$$\text{dist} \left(\sigma(\mathcal{H}_\varepsilon(\tau)), \Lambda_0 \right) \geq a\varepsilon \quad \text{for} \quad |\tau \pm \tau_0| \geq t_0(a)\varepsilon. \quad (3.2)$$

In other words, for the indicated values of τ the spectrum of $\mathcal{H}_\varepsilon(\tau)$ is separated from Λ_0 by a distance at least $A\varepsilon$, and it is now sufficient to study the band functions of \mathcal{H}_ε near Λ_0 as $|\tau \pm \tau_0| \leq t_0(a)\varepsilon$. We consider the case of τ_0 only; the case of $-\tau_0$ is studied in the same way.

We let $\tau = \tau_0 + \varepsilon t$, where $t \in [-t_0(a), t_0(a)]$ is a real-valued parameter. The number Λ_0 is a double eigenvalue of $\mathcal{H}_0(\tau_0)$, and the perturbation $\varepsilon \mathcal{L}_0(\tau_0 + \varepsilon t)$ is regular, see (2.2) and (2.3), and we can apply the standard regular perturbation theory, see e.g. [19, Ch. VII, §3]. The first of the estimates (3.1) shows that for sufficiently small $\varepsilon_0 > 0$ the operator $\mathcal{H}_\varepsilon(\tau_0 + \varepsilon t)$ has two eigenvalues (counting multiplicity) that converge to Λ_0 as $\varepsilon \rightarrow +0$. Denote these eigenvalues by $E_\pm(\varepsilon, \tau)$ and the associated eigenfunctions by $\phi_\pm(x, \tau, \varepsilon)$. Since the perturbation by $\varepsilon \mathcal{L}_0(\tau_0 + \varepsilon t)$ is regular and the operators $\mathcal{H}_\varepsilon(\tau_0 + \varepsilon t)$ are self-adjoint, the eigenvalues $E_\pm(\varepsilon, \tau + \varepsilon t)$ and the associated eigenfunctions $\phi_\pm(x, \tau + \varepsilon t, \varepsilon)$ are holomorph w.r.t. ε (the latter are holomorphic in $\dot{W}_{2,per}^2(\square)$ -norm), and the leading terms of their Taylor series near $\varepsilon = 0$ are of the form:

$$\begin{aligned} E_\pm(\varepsilon, \tau_0 + \varepsilon t) &= \Lambda_0 + \varepsilon K_\pm(t) + \mathcal{O}(\varepsilon^2), \\ \phi_\pm(x, t, \varepsilon) &= \Psi_\pm(x, t) + \varepsilon \Phi_\pm(x, t) + \mathcal{O}(\varepsilon^2), \\ \Psi_+ &:= c_1^+ \Psi_{j,p} + c_2^+ \Psi_{k,q}, \quad \Psi_- := c_1^- \Psi_{j,p} + c_2^- \Psi_{k,q}, \end{aligned} \quad (3.3)$$

where $c_i^\pm = c_i^\pm(t)$ are some constants that do not vanish simultaneously. Since the eigenfunctions ϕ_\pm can be chosen orthonormal in $L_2(\square)$, the same is true for Ψ_\pm . This gives

$$c_1^+ \overline{c_1^-} + c_2^+ \overline{c_2^-} = 0, \quad |c_1^\pm|^2 + |c_2^\pm|^2 = 1, \quad (3.4)$$

and the error estimates in (3.3) are uniform for $t \in [-t_0(a), t_0(a)]$ for any fixed a .

To determine the coefficients K_\pm it is sufficient to employ the regular perturbation theory. Namely, substitute the formulas (3.3) into the eigenvalue equation

$$\mathcal{H}_\varepsilon(\tau_0 + \varepsilon t)\phi_\pm = E_\pm \phi_\pm$$

and equate the coefficients at the first power of ε , then one arrives at the two equations

$$(\mathcal{H}_0(\tau_0) - \Lambda_0)\Phi_\pm = 2t l_n(\tau_0)\Psi_\pm + \mathcal{L}(\tau_0)\Psi_\pm + K_\pm \Psi_\pm.$$

These equations are solvable iff the functions at the right-hand side are orthogonal to $\Psi_{j,p}$ and $\Psi_{k,q}$ in $L_2(\square)$:

$$\begin{aligned} \langle 2t l_n(\tau_0)\Psi_\pm + \mathcal{L}(\tau_0)\Psi_\pm + K_\pm \Psi_\pm, \Psi_{j,p} \rangle_{L_2(\square)} &= 0, \\ \langle 2t l_n(\tau_0)\Psi_\pm + \mathcal{L}(\tau_0)\Psi_\pm + K_\pm \Psi_\pm, \Psi_{k,q} \rangle_{L_2(\square)} &= 0. \end{aligned} \quad (3.5)$$

Using the orthonormality of $\Psi_{j,p}$ and $\Psi_{k,q}$ and Eqs. (2.5) and (3.4) we arrive at

$$\begin{aligned} \langle l_n(\tau_0)\Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} &= \langle l_n(\tau_0)\Psi_{k,q}, \Psi_{j,p} \rangle_{L_2(\square)} = 0, \\ \langle l_n(\tau_0)\Psi_{j,p}, \Psi_{j,p} \rangle_{L_2(\square)} &= -\frac{2\pi p}{T} - \tau_0, \quad \langle l_n(\tau_0)\Psi_{k,q}, \Psi_{k,q} \rangle_{L_2(\square)} = -\frac{2\pi q}{T} - \tau_0 \end{aligned}$$

Thus, the solvability conditions (3.5) can be rewritten as

$$\begin{aligned} (B(t) - K_\pm(t))c_\pm(t) &= 0, \quad B(t) = 2tB_1 - B_0(\tau_0), \\ c_\pm &:= \begin{pmatrix} c_1^\pm \\ c_2^\pm \end{pmatrix}, \quad B_1 := \begin{pmatrix} \frac{2\pi p}{T} + \tau_0 & 0 \\ 0 & \frac{2\pi q}{T} + \tau_0 \end{pmatrix}. \end{aligned}$$

Therefore, K_\pm are the eigenvalues of $B(t)$, and $c_\pm(t)$ are the associated eigenvectors. By an explicit analysis,

$$K_\pm(t) = k_1(\tau_0)t + k_2(\tau_0) \pm \sqrt{(k_3(\tau_0)t + k_4(\tau_0))^2 + |b_{12}^0(\tau_0)|^2}, \quad (3.6)$$

with k_i given by (2.12). By (2.10) one has $K_+(t) > K_-(t)$ for all $t \in \mathbb{R}$. Using the explicit expressions again we obtain

$$2k_1(\tau_0) = -\frac{\partial \Lambda_{j,p}}{\partial \tau}(\tau_0) - \frac{\partial \Lambda_{k,q}}{\partial \tau}(\tau_0), \quad 2k_3(\tau_0) = \frac{\partial \Lambda_{j,p}}{\partial \tau}(\tau_0) - \frac{\partial \Lambda_{k,q}}{\partial \tau}(\tau_0).$$

In accordance with (2.8), the derivatives in the latter formulas have opposite signs, and this shows that

$$|k_1(\tau_0)| < |k_3(\tau_0)| \neq 0, \quad (3.7)$$

and implies the statement (A1). Together with (3.6) it yields

$$\lim_{|t| \rightarrow \infty} K_{\pm}(t) = \pm\infty. \quad (3.8)$$

By elementary consideration one can find the minimum of K_+ and the maximum of K_- ,

$$\begin{aligned} \min_{\mathbb{R}} K_+(t) &= K_+(t_+), \quad \max_{\mathbb{R}} K_-(t) = K_-(t_-), \\ t_{\pm} &= \mp \frac{k_1(\tau_0)|b_{12}^0(\tau_0)|}{|k_3(\tau_0)|\sqrt{k_3^2(\tau_0) - k_1^2(\tau_0)}} - \frac{k_4(\tau_0)}{k_3}, \quad K_{\pm}(t_{\pm}) = \beta_{\pm}(\tau_0), \end{aligned} \quad (3.9)$$

where β_{\pm} are given by (2.11). Let us choose the parameter a in (3.2) large enough and employ the asymptotics (3.3), then

$$\begin{aligned} \min_{\tau \in [0, \pi/T]} E_+(\varepsilon, \tau) &= \Lambda_0 + \varepsilon K_+(t_+) + \mathcal{O}(\varepsilon^2 + \varepsilon\eta), \\ \max_{\tau \in [0, \pi/T]} E_-(\varepsilon, \tau) &= \Lambda_0 + \varepsilon K_-(t_-) + \mathcal{O}(\varepsilon^2 + \varepsilon\eta), \end{aligned} \quad (3.10)$$

and $\max_{\tau \in [0, \pi/T]} E_-(\varepsilon, \tau) < \min_{\tau \in [0, \pi/T]} E_+(\varepsilon, \tau)$ for sufficiently small ε due to (3.9).

Similar arguments are valid for $\tau \in [-\pi/T, 0]$, and one arrives at the analogues of (3.3) and (3.9) near $-\tau_0$. To obtain the analogues of the expressions (2.13), (3.6), (3.7), (3.8), (3.9) and (3.10) one should just replace (p, q, τ_0) by $(-p, -q, -\tau_0)$ in (2.12) and (2.13), which gives exactly (2.14) and (2.16). This shows that $\mathcal{H}_{\varepsilon}$ there exists a gap $(\alpha_l(\varepsilon), \alpha_r(\varepsilon))$ with $\alpha_{l/r}(\varepsilon)$ given by (2.18).

The extrema of K_{\pm} are non-degenerate, $|K_{\pm}(t) - K_{\pm}(t_{\pm})| \geq C|t - t_{\pm}|^2$ with a t -independent constant C , and

$$|E_{\pm}(\varepsilon, \tau_0 + \varepsilon t) - \Lambda_0 - \varepsilon K_{\pm}(t_{\pm})| \geq C\varepsilon|t - t_{\pm}|^2 + \mathcal{O}(\varepsilon^2 + \varepsilon\eta).$$

This shows that the maximum points of $E_-(\varepsilon, \cdot)$ and the minimum points of $E_+(\varepsilon, \cdot)$ on $\tau \in [0, \pi/T]$ are separated from $\tau_0 + \varepsilon t_+$ and $\tau_0 + \varepsilon t_-$ by a distance of at most $\mathcal{O}(\varepsilon^{3/2} + \varepsilon\eta^{1/2})$, which proves the estimates (2.19) and (2.20) and completes the proof of the statement (A2).

To prove (A3) we remark first that $\Psi_{j,p} = \overline{\Psi_{j,-p}}$. If all the coefficients of the operator $\mathcal{H}_{\varepsilon}$ are real-valued, then it commutes with the complex conjugation. In particular, $\mathcal{L}_0(-\tau)\Psi_{j,-p} = \overline{\mathcal{L}_0(\tau)\Psi_{j,p}}$, and $\beta_{\pm}(\tau_0) = \beta_{\pm}(-\tau_0)$. Now the validity of (2.17) follows trivially from (A1).

In the case $\tau_0 = 0$ the condition (2.17) is reduced to the strict inequality $\beta_-(0) < \beta_+(0)$, which is true due to (A1). Theorem 2.1 is proved.

4. EXAMPLES

Let us discuss in greater detail several specific situations to which one can apply Theorem 2.1. We will focus mainly on checking the conditions (2.10) and (2.17).

4.1. Potential. Adding a real-valued periodic potential may be viewed as one of the simplest examples. One has simply $\mathcal{L}_{\varepsilon} = A_0$. In accordance with the conclusion (A3) it is sufficient to check the condition (2.10), which loses the dependence on τ_0 and looks very simple,

$$\langle A_0 \Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} \equiv \int_{\square} A_0(x) \psi_j(x') \psi_k(x') e^{2\pi i(p-q)x_n/T} dx \neq 0.$$

This inequality is satisfied by a large class of potentials, and we can conclude that a generic potential perturbation opens the described gap in the spectrum as far as the cross-section and the period obey the relations discussed in Remark 2.2.

4.2. Magnetic field. Another natural perturbation is the action of a weak magnetic field. The perturbed operator has the form $\mathcal{H}_\varepsilon = (\mathbf{i}\nabla + \varepsilon A)^2$, where $A = (A_1, \dots, A_n)$ is magnetic vector potential, and the perturbing operator is given by

$$\mathcal{L}_\varepsilon := \mathbf{i} \sum_{i=1}^n \left(A_i \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i} A_i \right) + \varepsilon |A|^2.$$

This results in

$$\mathcal{L}_0(\tau) = \mathbf{i} \sum_{i=1}^n \left(A_i \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i} A_i \right) - 2\tau A_n.$$

For $\tau \geq 0$ we calculate the entries of the matrix $B_0(\tau)$ using the integration by parts

$$\begin{aligned} b_{12}^0(\tau) &= \overline{b_{21}^0(\tau)} = \mathbf{i} \sum_{i=1}^n \left(\left\langle A_i \frac{\partial \Psi_{j,p}}{\partial x_i}, \Psi_{k,q} \right\rangle_{L_2(\square)} - \left\langle A_i \Psi_{j,p}, \frac{\partial \Psi_{k,q}}{\partial x_i} \right\rangle_{L_2(\square)} \right) \\ &\quad - 2\tau \langle A_n \Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} \\ &= \frac{\mathbf{i}}{T} \sum_{i=1}^{n-1} \int_{\square} e^{\frac{2\pi \mathbf{i}(p-q)}{T} x_n} A_i(x) \left(\frac{\partial \psi_j}{\partial x_i}(x') \psi_k(x') - \frac{\partial \psi_k}{\partial x_i}(x') \psi_j(x') \right) dx \\ &\quad - \frac{2}{T} \left(\frac{\pi(p+q)}{T} + \tau \right) \int_{\square} e^{\frac{2\pi \mathbf{i}(p-q)}{T} x_n} A_n(x) \psi_j(x') \psi_k(x') dx, \\ b_{11}^0(\tau) &= -\frac{2}{T} \left(\frac{2\pi p}{T} + \tau \right) \int_{\square} A_n(x) \psi_j^2(x') dx, \\ b_{22}^0(\tau) &= -\frac{2}{T} \left(\frac{2\pi p}{T} + \tau \right) \int_{\square} A_n(x) \psi_k^2(x') dx. \end{aligned} \quad (4.1)$$

Similar calculations for $\tau < 0$ give the relations

$$b_{im}^0(-\tau) = -\overline{b_{mi}^0(\tau)}, \quad i, m = 1, 2, \quad k_i(-\tau) = -k_i(\tau), \quad i = 2, 4, \quad (4.2)$$

and

$$\beta_{\pm}(-\tau) = -\beta_{\mp}(\tau). \quad (4.3)$$

Taking into account (A1) one can see that the condition (2.17) becomes equivalent to $\beta_+(\tau_0) > \beta_-(-\tau_0)$ and $\beta_-(-\tau_0) > \beta_+(\tau_0)$. By (4.3) this reduces to

$$\pm \beta_{\pm}(\tau_0) > 0, \quad (4.4)$$

which is an equivalent compact form for (2.17).

Since p and q must have opposite signs (see Remark 2.2), one may assume without loss of generality $p \geq 0$ and $q < 0$, then the function $k_3(\tau_0)$ becomes positive. Substituting (2.11), (2.12) and (4.1) into (4.4) one arrives at

$$\begin{aligned} |b_{12}^0(\tau_0)| \sqrt{k_3^2(\tau_0) - k_1^2(\tau_0)} &> |k_1(\tau_0)k_4(\tau_0) - k_3(\tau_0)k_2(\tau_0)|, \\ |b_{12}^0(\tau_0)| \sqrt{k_3^2(\tau_0) - k_1^2(\tau_0)} &> \left| a_{11} \left(\frac{2\pi p}{T} + \tau_0 \right)^2 - a_{22} \left(\frac{2\pi q}{T} + \tau_0 \right)^2 \right|, \end{aligned} \quad (4.5)$$

$$\text{where } a_{11} := \frac{1}{T} \int_{\square} A_n(x) \psi_j^2(x') dx \text{ and } a_{22} := \frac{1}{T} \int_{\square} A_n(x) \psi_k^2(x') dx. \quad (4.6)$$

These inequalities together with

$$b_{12}^0(\tau_0) \neq 0 \quad (4.7)$$

give the final set of sufficient conditions guaranteeing the existence of a gap for \mathcal{H}_ε .

Let us now give an example of a specific magnetic field satisfying (4.5) and (4.7). We restrict our attention to the functions $A_n(x)$ obeys

$$\int_0^T A_n(x) dx_n = 0 \quad \text{for all } x' \in \omega,$$

then (4.6) shows that $a_{11} = a_{22} = 0$, and the inequality (4.5) is satisfied once the condition (4.7) is valid. Assume additionally $A_1(x) \equiv A_2(x) \equiv \dots \equiv A_{n-1}(x) \equiv 0$, then the expression (4.1) for b_{12}^0 can be considerably simplified, and Eq. (4.7) becomes equivalent to

$$\left(\frac{\pi(p+q)}{T} + \tau_0 \right) \int_{\omega} dx' \psi_q(x') \psi_p(x') \int_0^T dx_n A_n(x) e^{\frac{2\pi i(p-q)}{T} x_n} \neq 0.$$

For $\tau_0 = 0$ and $\tau_0 = \pi/T$ the coefficient before the integral vanishes, see Remark 2.2, and our constructions do not allow to identify the gap opening (if a gap opens, its length is of order $o(\varepsilon)$). On the other hand, for $\tau_0 \in (0, \pi/T)$ the coefficient is non-zero, and all the required conditions are satisfied if one takes

$$A_n(x) = \psi_1(x') \psi_2(x') \varphi_1(x') \cos \frac{2\pi(p-q)}{T} x_n + \varphi_2(x),$$

where $\varphi_1 \in C^1(\overline{\omega})$ is an arbitrary positive function and $\varphi_2 \in C^1(\overline{\Omega})$ is an arbitrary T -periodic w.r.t. x_n function satisfying the condition

$$\int_0^T \varphi_2(x) dx_n = \int_0^T e^{\frac{2\pi(p-q)}{T} x_n} \varphi_2(x) dx_n = 0 \quad \text{for all } x' \in \omega.$$

For instance, one take simply $\varphi_1 \equiv 1$ and $\varphi_2 \equiv 0$. Thus we can conclude that the magnetic field can open a gap corresponding to the values of the quasi-momentum different from 0 and $\pm\pi/T$.

4.3. Deformation of boundary. Let us study a geometric perturbation consisting a periodic deformation of the boundary. We consider the two-dimensional strip

$$\Omega_\varepsilon := \{(y_1, y_2) : \varepsilon h_-(y_2) < y_1 < 1 + \varepsilon h_+(y_2)\}, \quad y = (y_1, y_2),$$

where h_\pm are smooth T -periodic functions. Denote by $\tilde{\mathcal{H}}_\varepsilon$ the positive Dirichlet Laplacian in Ω_ε . Let us show that such operators are covered by the aforementioned construction. Let us denote $h := h_+ - h_-$. For small ε the map $\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$,

$$\Phi_\varepsilon(x_1, x_2) = \begin{pmatrix} \varepsilon h_-(x_2) + (1 + \varepsilon h(x_2)) x_1 \\ x_2 \end{pmatrix}$$

is the diffeomorphism, and $\Omega_\varepsilon = \Phi_\varepsilon(\Omega_0)$. Let $J\Phi_\varepsilon$ be the Jacobi matrix of Φ_ε , then the map

$$U_\varepsilon : L_2(\Omega_\varepsilon) \rightarrow L_2(\Omega_0), \quad U_\varepsilon f = \sqrt{\det J\Phi_\varepsilon} f \circ \Phi_\varepsilon, \quad (4.8)$$

is unitary, and the operator $\mathcal{H}_\varepsilon := U_\varepsilon \tilde{\mathcal{H}}_\varepsilon U_\varepsilon^*$ corresponds to the sesquilinear form

$$q_\varepsilon(u, v) = \int_{\Omega_0} \nabla \left(\frac{u(x)}{\sqrt{\det J\Phi_\varepsilon(x)}} \right) \cdot (J\Phi_\varepsilon^t \cdot J\Phi_\varepsilon)^{-1} \nabla \left(\frac{\overline{v(x)}}{\sqrt{\det J\Phi_\varepsilon(x)}} \right) \det J\Phi_\varepsilon(x) dx, \quad (4.9)$$

i.e.,

$$\mathcal{H}_\varepsilon = -\frac{1}{\det J\Phi_\varepsilon} \operatorname{div} \left(\det J\Phi_\varepsilon (J\Phi_\varepsilon^t \cdot J\Phi_\varepsilon)^{-1} \nabla \frac{1}{\sqrt{\det J\Phi_\varepsilon}} \right).$$

In our case

$$J\Phi_\varepsilon(x_1, x_2) = \begin{pmatrix} 1 + \varepsilon h(x_2) & \varepsilon(h'_-(x_2) + x_1 h(x_2)) \\ 0 & 1 \end{pmatrix},$$

which shows that \mathcal{H}_ε has real-valued coefficients and has the required representation $\mathcal{H}_\varepsilon = \mathcal{H}_0 + \varepsilon \mathcal{L}_\varepsilon$. By direct calculation we get

$$\begin{aligned} \langle \mathcal{L}_0 u, v \rangle_{L_2(\mathbb{R}^2)} &= - \int_{\Omega_0} \frac{h'(x_2)}{2} \left[u(x) \frac{\partial v(x)}{\partial x_2} + \frac{\partial u(x)}{\partial x_2} \overline{v(x)} \right] + 2h(x_2) \frac{\partial u(x)}{\partial x_1} \frac{\partial v(x)}{\partial x_1} \\ &\quad + (h'_-(x_2) + x_1 h'(x_2)) \left(\frac{\partial u(x)}{\partial x_1} \frac{\partial v(x)}{\partial x_2} + \frac{\partial u(x)}{\partial x_2} \frac{\partial v(x)}{\partial x_1} \right) dx. \end{aligned}$$

Let us find a class of functions h_\pm for which the matrix entry (2.10) is non-zero. The transversal orthonormal eigenfunctions ψ_j are given by the explicit expressions $\psi_j(x) = \sqrt{2} \sin(\pi j x)$, $j = 1, 2, \dots$. Employing the notation

$$\hat{h}_m = \int_0^T e^{2\pi i m x_2 / T} h(x_2) dx_2,$$

by direct calculations we obtain

$$I := \langle \mathcal{L}_0(\tau_0) \Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} = \langle \mathcal{L}_0 \Psi_{j,p} e^{i\tau_0 x_2}, \Psi_{k,q} e^{i\tau_0 x_2} \rangle_{L_2(\square)} = -\frac{I_1 + I_2 + I_3}{T},$$

where

$$\begin{aligned} I_1 &= \frac{1}{2} \int_{\square} \frac{2\pi i(p-q)}{T} h'(x_2) e^{2\pi i(p-q)x_2/T} \psi_j(x_1) \psi_k(x_1) dx = \frac{2\pi^2(p-q)^2}{T^2} \hat{h}_{p-q} \delta_{jk}, \\ I_2 &= 2 \int_{\square} h(x_2) e^{2\pi i(p-q)x_2/T} \psi'_j(x_1) \psi'_k(x_1) dx = 2(\pi j)^2 \hat{h}_{p-q} \delta_{jk}, \\ I_3 &= i \int_{\square} (h'_-(x_2) + x_1 h'(x_2)) e^{2\pi i(p-q)x_2/T} \\ &\quad \cdot \left(\left(\tau_0 + \frac{2\pi p}{T} \right) \psi_j(x_1) \psi'_k(x_1) - \left(\tau_0 + \frac{2\pi q}{T} \right) \psi'_j(x_1) \psi_k(x_1) \right) dx. \end{aligned}$$

We observe that for $j, k \in \mathbb{N}$ one has

$$\begin{aligned} \int_0^1 \psi_j(x_1) \psi'_k(x_1) dx_1 &= \begin{cases} 0, & j = k, \\ (1 + (-1)^{j+k+1}) \frac{2jk}{j^2 - k^2}, & j \neq k, \end{cases} \\ \int_0^1 x_1 \psi_j(x_1) \psi'_k(x_1) dx_1 &= \begin{cases} \frac{1}{2}, & j = k, \\ (-1)^{j+k+1} \frac{2jk}{j^2 - k^2}, & j \neq k. \end{cases} \end{aligned}$$

Let us consider first the symmetric intersection $\tau_0 = 0$. This implies immediately $q = -p$, $j = k = 1$,

$$I_3 = \frac{2\pi i p}{T} \int_0^T h'(x_2) e^{4\pi i p x_2 / T} dx_1 = \frac{8\pi^2 p^2}{T^2} \hat{h}_{2p},$$

and

$$I = -\frac{1}{T} \left(\frac{16\pi^2 p^2}{T^2} + 2\pi^2 \right) \hat{h}_{2p}.$$

Thus, the condition $\hat{h}_{2p} \neq 0$ is sufficient to satisfy (2.10).

For $\tau_0 = \pi/T$ we have $j = k = 1$ and $q = -p - 1$ and

$$I = -\frac{1}{T} \left(\frac{4\pi^2(2p+1)^2}{T^2} + 2\pi^2 \right) \hat{h}_{2p+1},$$

so the condition (2.10) holds true for $\hat{h}_{2p+1} \neq 0$.

Let us consider the non-symmetric case $\tau_0 \in (0, \pi/T)$. Without loss of generality we let $j = 1$ and $k = 2$. It implies immediately that $I_1 = I_2 = 0$. On the other hand, by using (2.21) we get

$$\begin{aligned} I_3 &= -\frac{2i}{3} \left(2\tau_0 + \frac{2\pi(p+q)}{T} \right) \int_0^T \left(2h'_-(x_2) + h'(x_2) \right) e^{2\pi i(p-q)x_2/T} dx_2 \\ &= \frac{2i}{3} \left(2\tau_0 + \frac{2\pi(p+q)}{T} \right) \int_0^T \left(h'_-(x_2) + h'_+(x_2) \right) e^{2\pi i(p-q)x_2/T} dx_2 \\ &= \frac{2}{3} \frac{2\pi(p-q)}{T} \left(\frac{2\pi(p+q)}{T} + 2\tau_0 \right) \widehat{(h_- + h_+)}_{p-q} \\ &= 2\pi^2 \widehat{(h_- + h_+)}_{p-q}. \end{aligned}$$

Thus, the condition (2.10) holds true as $\widehat{(h_- + h_+)}_{p-q} \neq 0$.

It is an interesting fact that for $\tau_0 = 0$ and $\tau_0 = \pi/T$ the sufficient conditions for a gap opening are formulated in terms of the Fourier coefficients of the function $h := h_+ - h_-$, while for $\tau_0 \in (0, \pi/T)$ the same role is played by the function $h_+ + h_-$. In other words, for $\tau_0 = 0$ and $\tau_0 = \pi/T$ the gap opening is controlled, at the first order, by the strip width, while for $\tau \in (0, \pi/T)$ the same role is played by the sum of the side variations.

4.4. Three-dimensional rod with a periodic twisting. Let $\theta : \mathbb{R} \rightarrow \mathbb{R}$ be a smooth T -periodic function. For $\varepsilon > 0$ consider a diffeomorphism $\Phi_\varepsilon : \mathbb{R}^3 \rightarrow \mathbb{R}^3$,

$$\Phi_\varepsilon(x_1, x_2, x_3) = \begin{pmatrix} \cos(\varepsilon\theta(x_3))x_1 - \sin(\varepsilon\theta(x_3))x_2 \\ \sin(\varepsilon\theta(x_3))x_1 + \cos(\varepsilon\theta(x_3))x_2 \\ x_3 \end{pmatrix},$$

and denote by ω we denote a two-dimensional connected domain with a piece-smooth Lipschitz boundary. Let $\Omega_0 := \omega \times \mathbb{R}$ and $\Omega_\varepsilon := \Phi_\varepsilon(\Omega_0)$. For $\varepsilon = 0$ we just get a straight cylinder with a constant cross-section ω , while for $\varepsilon \neq 0$ the cross-section is rotated around the axis Oy_3 by the angle $\varepsilon\theta(y_3)$ w.r.t. the initial position in each plane $y_3 = \text{const}$.

Let us denote by $\tilde{\mathcal{H}}_\varepsilon$ the Dirichlet Laplacian in Ω_ε . By analogy with (4.9) one can show that this geometric perturbation can be reduced to an additive perturbation. Since these constructions were already discussed in various contexts, we employ the ready expression for the perturbing operator obtained in [20, Eq. (15)]. Denote $\mathcal{H}_\varepsilon := U_\varepsilon \tilde{\mathcal{H}}_\varepsilon U_\varepsilon^*$ with the unitary U_ε given by (4.8), then, for any $u, v \in W_2^2(\Omega)$,

$$\langle \mathcal{H}_\varepsilon u, v \rangle_{L_2(\Omega)} = \int_\Omega \nabla u(x) \cdot G_\varepsilon(x) \nabla \overline{v(x)} dx, \quad (4.10)$$

where

$$G_\varepsilon(x) = \begin{pmatrix} 1 + (\varepsilon x_2 \theta'(x_3))^2 & -\varepsilon^2 x_1 x_2 (\theta'(x_3))^2 & \varepsilon x_2 \theta'(x_3) \\ -\varepsilon^2 x_1 x_2 (\theta'(x_3))^2 & 1 + (\varepsilon x_1 \theta'(x_3))^2 & -\varepsilon x_1 \theta'(x_3) \\ \varepsilon x_2 \theta'(x_3) & -\varepsilon x_1 \theta'(x_3) & 0 \end{pmatrix}.$$

Thus, $\mathcal{H}_\varepsilon = -\Delta + \varepsilon \mathcal{L}_\varepsilon$, where the perturbation \mathcal{L}_ε satisfies all the required conditions, and its leading term \mathcal{L}_0 is given by

$$\begin{aligned} \langle \mathcal{L}_0 u, v \rangle_{L_2(\Omega)} &= \int_{\Omega} \theta'(x_3) x_2 \left(\frac{\partial u}{\partial x_1}(x) \overline{\frac{\partial v}{\partial x_3}}(x) + \frac{\partial u}{\partial x_3} \overline{\frac{\partial v}{\partial x_1}}(x) \right) \\ &\quad - \theta'(x_3) x_1 \left(\frac{\partial u}{\partial x_2}(x) \overline{\frac{\partial v}{\partial x_3}}(x) + \frac{\partial u}{\partial x_3} \overline{\frac{\partial v}{\partial x_2}}(x) \right) dx. \end{aligned}$$

We note that \mathcal{H}_ε commutes with the complex conjugation, and it remains to find the conditions guaranteeing the validity of (2.10). There holds

$$\begin{aligned} I &:= \langle \mathcal{L}_0(\tau_0) \Psi_{j,p}, \Psi_{k,q} \rangle_{L_2(\square)} = \langle \mathcal{L}_0 \Psi_{j,p} e^{i\tau_0 x_3}, \Psi_{k,q} e^{i\tau_0 x_3} \rangle_{L_2(\square)} \\ &= \frac{1}{T} \int_{\Omega} \theta'(x_3) x_2 e^{2\pi i(p-q)x_3/T} \\ &\quad \cdot \left[-i \left(\frac{2\pi q}{T} + \tau_0 \right) \frac{\partial \psi_j}{\partial x_1}(x_1, x_2) \psi_k(x_1, x_2) + i \left(\frac{2\pi p}{T} + \tau_0 \right) \psi_j(x_1, x_2) \frac{\partial \psi_k}{\partial x_1}(x_1, x_2) \right] \\ &\quad - \theta'(x_3) x_1 e^{2\pi i(p-q)x_3/T} \\ &\quad \cdot \left[-i \left(\frac{2\pi q}{T} + \tau_0 \right) \frac{\partial \psi_j}{\partial x_2}(x_1, x_2) \psi_k(x_1, x_2) + i \left(\frac{2\pi p}{T} + \tau_0 \right) \psi_j(x_1, x_2) \frac{\partial \psi_k}{\partial x_2}(x_1, x_2) \right] dx \\ &= a(b - c), \end{aligned}$$

where

$$\begin{aligned} a &= \frac{i}{T} \int_0^T \theta'(x_3) e^{2\pi i(p-q)x_3/T} dx_3 = \frac{2\pi(p-q)}{T^2} \int_0^T \theta(x_3) e^{2\pi i(p-q)x_3/T} dx_3, \\ b &= i \left(\frac{2\pi p}{T} + \tau_0 \right) \int_{\omega} x_2 \left(\psi_j \frac{\partial \psi_k}{\partial x_1} + \frac{\partial \psi_j}{\partial x_1} \psi_k \right) dx_1 dx_2 \\ &\quad - i \left(\frac{2\pi p}{T} + \tau_0 \right) \int_{\omega} x_1 \left(\psi_j \frac{\partial \psi_k}{\partial x_2} + \frac{\partial \psi_j}{\partial x_2} \psi_k \right) dx_1 dx_2, \\ c &= \left(\frac{2\pi(p+q)}{T} + 2\tau_0 \right) \int_{\omega} \left(x_2 \frac{\partial \psi_j}{\partial x_1} \psi_k - x_1 \frac{\partial \psi_j}{\partial x_2} \psi_k \right) dx_1 dx_2. \end{aligned}$$

One observes that the coefficient a does not depend on the cross-section and can be chosen non-zero by an appropriate choice of the twisting function θ . The Green's formula gives the identities

$$\begin{aligned} \int_{\omega} x_2 \left(\psi_j \frac{\partial \psi_k}{\partial x_1} + \frac{\partial \psi_j}{\partial x_1} \psi_k \right) dx_1 dx_2 &= \int_{\omega} x_2 \frac{\partial}{\partial x_1} (\psi_j \psi_k) dx_1 dx_2 = \int_{\partial\omega} x_2 \psi_j \psi_k dx_2, \\ \int_{\omega} x_1 \left(\psi_j \frac{\partial \psi_k}{\partial x_2} + \frac{\partial \psi_j}{\partial x_2} \psi_k \right) dx_1 dx_2 &= \int_{\omega} x_1 \frac{\partial}{\partial x_2} (\psi_j \psi_k) dx_1 dx_2 = - \int_{\partial\omega} x_1 \psi_j \psi_k dx_1. \end{aligned}$$

Since the both functions ψ_j and ψ_k vanish at the boundary $\partial\omega$, one has

$$\int_{\partial\omega} x_1 \psi_j \psi_k dx_1 = \int_{\partial\omega} x_2 \psi_j \psi_k dx_2 = 0$$

which gives $b \equiv 0$.

Let us study the remaining coefficient c . In the case of a symmetric intersection of the unperturbed band functions, i.e., for $\tau_0 = 0$ or $\tau = \pi/T$, we have $j = k$ and $p \neq q$, which implies by (2.21) that $c = 0$ and $I = 0$. Therefore, the assumptions of Theorem 2.1 are not satisfied, and the first order perturbation theory does not allow us to identify a gap opening for quasi-momenta close to the center and to the end points of the Brillouin zone.

For $\tau_0 \notin (0, \pi/T)$ we have $j \neq k$ and $p \neq -q$, and by (2.21) we conclude that $p + q + 2\tau_0 \neq 0$. Let us show that the integral entering the expression for c does not vanish at least for some specific domains ω . Without loss of generality we let $j = 1$ and $k = 2$, and take as an example $\omega = (0, \pi) \times (0, \pi/\alpha)$ with $\alpha > 1$. Denoting $C = 2\sqrt{\alpha}/\pi$, we have

$$\begin{aligned}\lambda_1 &= 1 + \alpha^2, & \psi_1(x_1, x_2) &= C \sin(x_1) \sin(\alpha x_2), \\ \lambda_2 &= 4 + \alpha^2, & \psi_2(x_1, x_2) &= C \sin(2x_1) \sin(\alpha x_2),\end{aligned}$$

and

$$\frac{\partial \psi_1}{\partial x_1}(x_1, x_2) = C \cos(x_1) \sin(\alpha x_2), \quad \frac{\partial \psi_1}{\partial x_2}(x_1, x_2) = \alpha C \sin(x_1) \cos(\alpha x_2).$$

It yields

$$\begin{aligned}x_2 \frac{\partial \psi_1}{\partial x_1} \psi_2 &= \frac{C^2}{4} x_2 (\sin(3x_1) + \sin(x_1)) \cdot (1 - \cos(2\alpha x_2)), \\ x_1 \frac{\partial \psi_1}{\partial x_2} \psi_2 &= \frac{\alpha C^2}{4} x_1 (\cos(x_1) - \cos(3x_1)) \cdot \sin(2\alpha x_2),\end{aligned}$$

and

$$\begin{aligned}\int_{\omega} x_2 \frac{\partial \psi_1}{\partial x_1} \psi_2 \, dx_1 \, dx_2 &= \frac{C^2}{4} \int_0^{\pi} (\sin(3x_1) + \sin(x_1)) \, dx_1 \cdot \int_0^{\pi/\alpha} x_2 (1 - \cos(2\alpha x_2)) \, dx_2 \\ &= \frac{\alpha}{\pi^2} \frac{8}{3} \frac{\pi^2}{2\alpha^2} = \frac{4}{3\alpha}, \\ \int_{\omega} x_1 \frac{\partial \psi_1}{\partial x_2} \psi_2 \, dx_1 \, dx_2 &= \frac{\alpha C^2}{4} \int_0^{\pi} x_1 (\cos(x_1) - \cos(3x_1)) \, dx_1 \int_0^{\pi/\alpha} \sin(2\alpha x_2) \, dx_2 = 0.\end{aligned}$$

Finally, by employing (2.21) we obtain

$$\begin{aligned}I &= -ac = -\left(\frac{2\pi(p+q)}{T} + 2\tau_0\right) \frac{4}{3\alpha} \frac{2\pi(p-q)}{T^2} \int_0^T \theta(x_3) e^{2\pi i(p-q)x_3/T} \, dx_3 \\ &= -\frac{4\pi^2}{\alpha T} \int_0^T \theta(x_3) e^{2\pi i(p-q)x_3/T} \, dx_3,\end{aligned}$$

and $I \neq 0$, if the Fourier coefficient in the previous expression is non-zero.

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